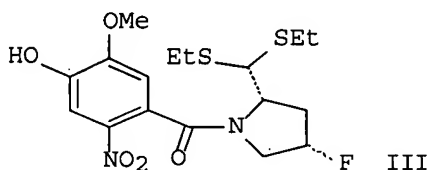
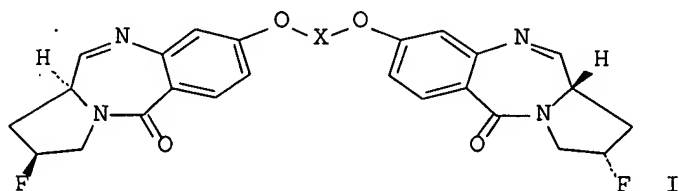


L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:1078234 CAPLUS Full-text  
 DN 143:347210  
 TI A preparation of fluoropyrrolobenzodiazepine dimers, useful as antitumor agents  
 IN Kamal, Ahmed; Reddy, Peram Surakattula Murali Mohan; Reddy, Depatla Rajashekhar  
 PA Council of Scientific and Industrial Research, India  
 SO U.S. Pat. Appl. Publ., 13 pp.  
 CODEN: USXXCO  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005222131	A1	20051006	US 2004-812840	20040330
PRAI	US 2004-812840		20040330		

GI



AB The invention relates to a preparation of fluoropyrrolobenzodiazepine dimers of formula I [wherein: X is (CH<sub>2</sub>)<sub>3-10</sub>], useful as antitumor agents. For instance, fluoropyrrolobenzodiazepine dimer II (I, X = (CH<sub>2</sub>)<sub>4</sub>; logGI<sub>50</sub> = -5.21, logTGI<sub>50</sub> = -4.75) was prepared from diethylthioacetal derivative III via 3 steps.

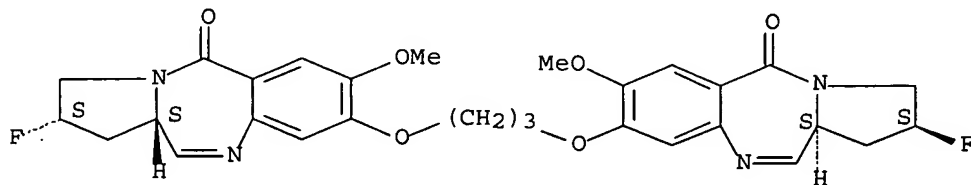
IT 717920-82-6P 717920-83-7P 717920-84-8P  
 858639-17-5P 858639-19-7P 858639-21-1P  
 858639-23-3P 858639-25-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoropyrrolobenzodiazepine dimers useful as antitumor agents)

RN 717920-82-6 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

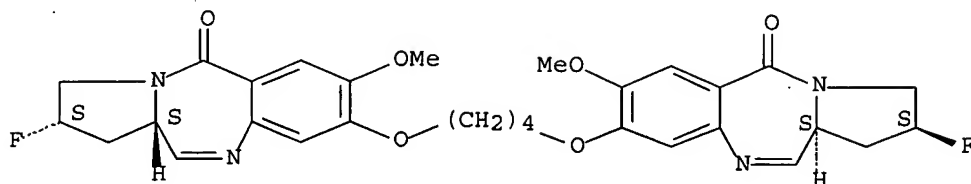


RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-,

(2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

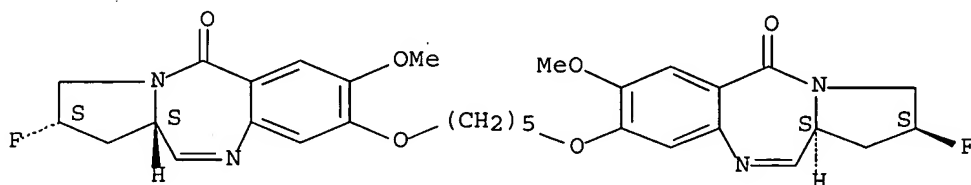
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

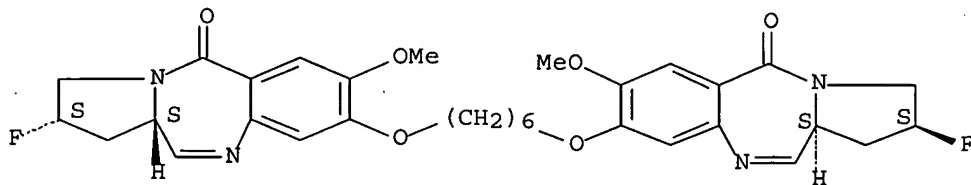
Absolute stereochemistry.



RN 858639-17-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,6-hexanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

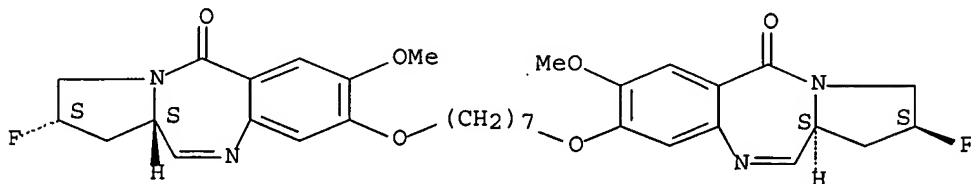
Absolute stereochemistry.



RN 858639-19-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,7-heptanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

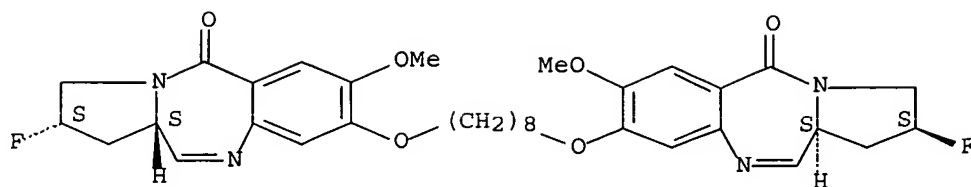
Absolute stereochemistry.



RN 858639-21-1 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,8-octanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

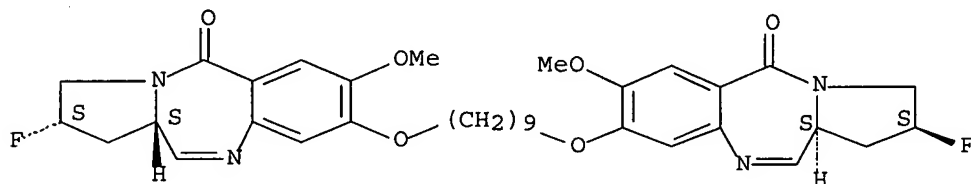
Absolute stereochemistry.



RN 858639-23-3 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,9-nonanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

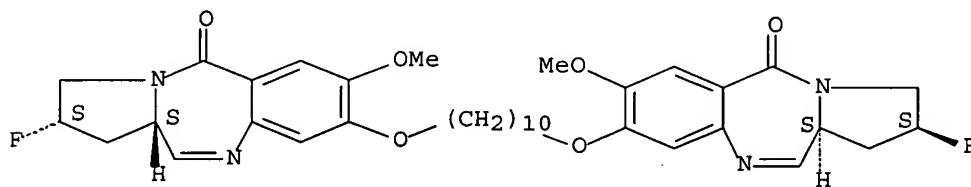
Absolute stereochemistry.



RN 858639-25-5 CAPLUS

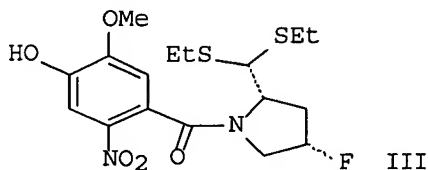
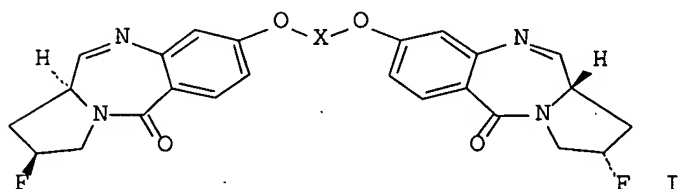
CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,10-decanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



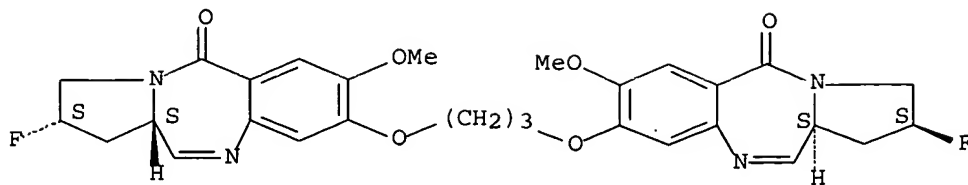
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:612296 CAPLUS Full-text  
 DN 143:133404  
 TI A preparation of fluoropyrrolobenzodiazepine dimers, useful as antitumor agents  
 IN Kamal, Ahmed; Reddy, Peram Surakattula Murali Mohan; Reddy, Depatla Rajasekhar  
 PA Council of Scientific and Industrial Research, India  
 SO PCT Int. Appl., 28 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005063758	A1	20050714	WO 2003-IN448	20031231
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PRAI	WO 2003-IN448		20031231		
OS	CASREACT 143:133404				
GI					



AB The invention relates to a preparation of fluoropyrrolobenzodiazepine dimers of formula I [wherein: X is (CH<sub>2</sub>)<sub>3-10</sub>], useful as antitumor agents. For instance, fluoropyrrolobenzodiazepine dimer II (I, X = CH<sub>2</sub>)<sub>4</sub>; (logGI<sub>50</sub> = -5.21, logTGI<sub>50</sub> = -4.75) was prepared from diethylthioacetal derivative III via 3 steps.  
 IT 717920-82-6P 717920-83-7P 717920-84-8P  
 858639-17-5P 858639-19-7P 858639-21-1P  
 858639-23-3P 858639-25-5P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoropyrrolobenzodiazepine dimers useful as antitumor agents)  
 RN 717920-82-6 CAPLUS  
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

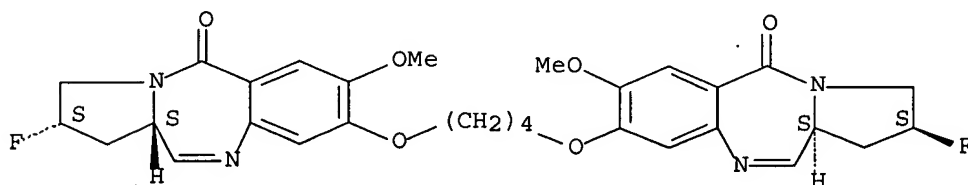
Absolute stereochemistry.



RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

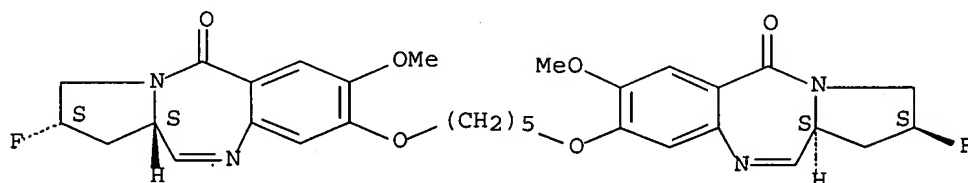
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediybis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

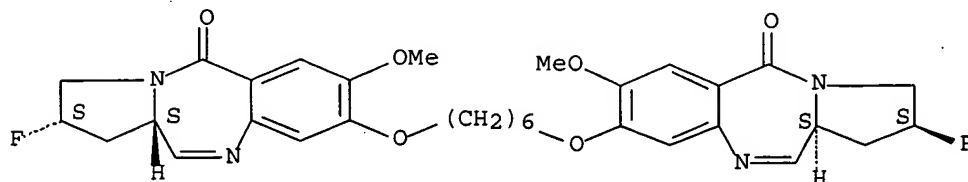
Absolute stereochemistry.



RN 858639-17-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,6-hexanediybis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

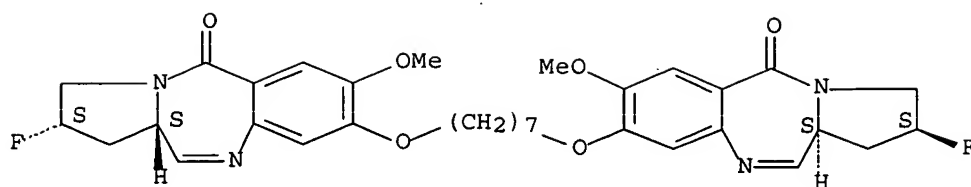
Absolute stereochemistry.



RN 858639-19-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,7-heptanediybis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

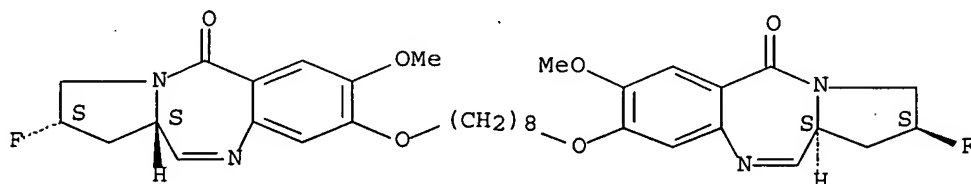
Absolute stereochemistry.



RN 858639-21-1 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,8-octanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

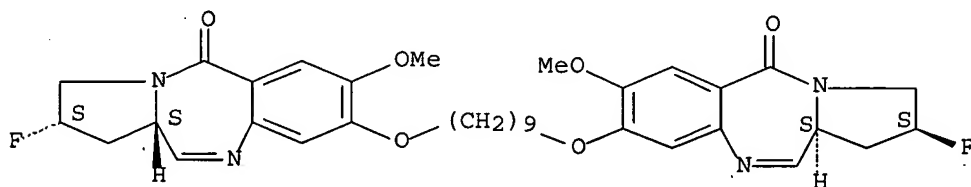
Absolute stereochemistry.



RN 858639-23-3 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,9-nonanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

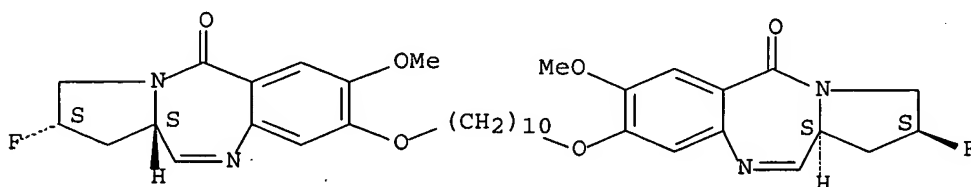
Absolute stereochemistry.



RN 858639-25-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,10-decanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

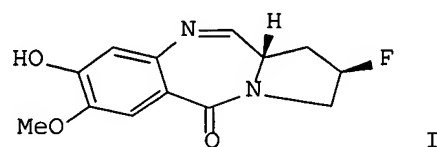
Absolute stereochemistry.



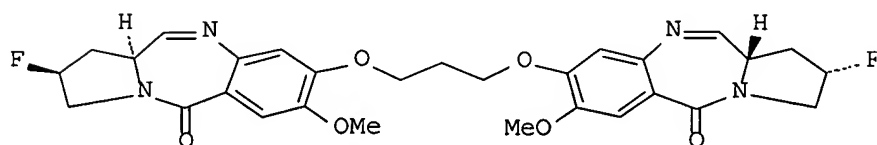
RE.CNT 4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2004:346285 CAPLUS Full-text.  
 DN 141:106440  
 TI The effect of C2-fluoro group on the biological activity of DC-81 and its dimers  
 AU Kamal, Ahmed; Reddy, P. S. M. M.; Reddy, D. Rajasekhara  
 CS Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500007, India  
 SO Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2669-2672  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 OS CASREACT 141:106440  
 GI



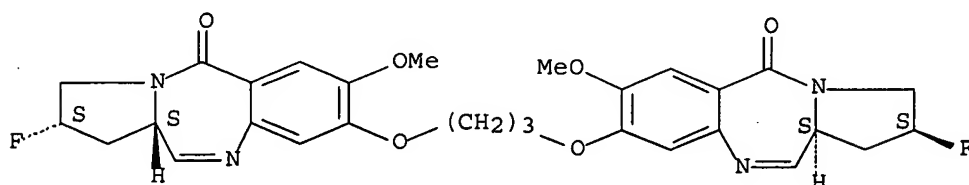
I



II

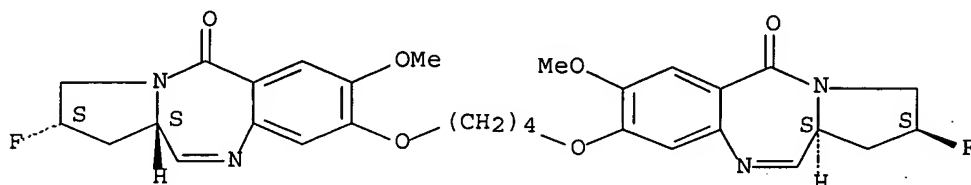
AB C2-Fluoro substituted pyrrolobenzodiazepines were synthesized that exhibit potential anticancer activity in a number of human tumor cell lines. These C2-fluoro substituted PBDs also exhibit significant DNA-binding ability. Example compds. included (2R,11aS)-2-Fluoro-1,2,3,11a-tetrahydro-8-hydroxy-7-methoxy-5H-pyrrolo[2,1-c][1,4]benzodiazepin-5-one (I) and a dimer (II).  
 IT 717920-82-6P 717920-83-7P 717920-84-8P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of (fluoro)tetrahydro(hydroxy)pyrrolo[2,1-c][1,4]benzodiazepin-5-one derivs. and dimers and study of their anticancer activity)  
 RN 717920-82-6 CAPLUS  
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



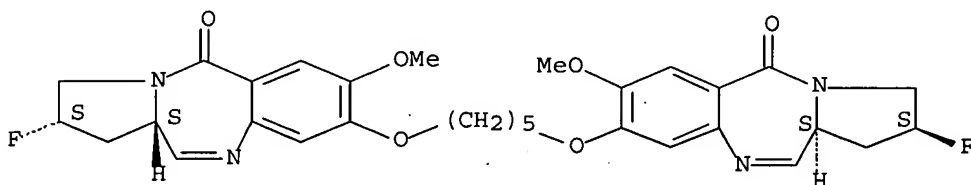
RN 717920-83-7 CAPLUS  
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 717920-84-8 CAPLUS  
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediylobis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 L4 8 S L2 FUL

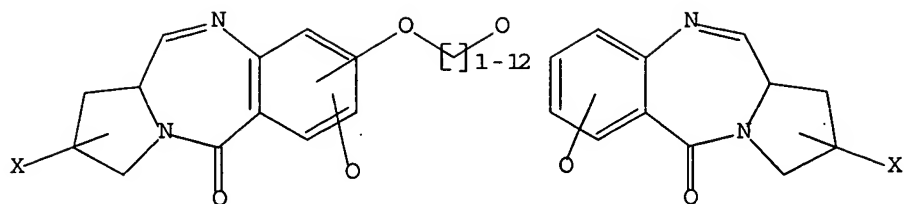
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L5 3 S L4

=> d l2; d his

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.  
 L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 09:33:29 ON 27 JAN 2006)

FILE 'REGISTRY' ENTERED AT 09:34:02 ON 27 JAN 2006

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 L3 1 S L2  
 L4 8 S L2 FUL

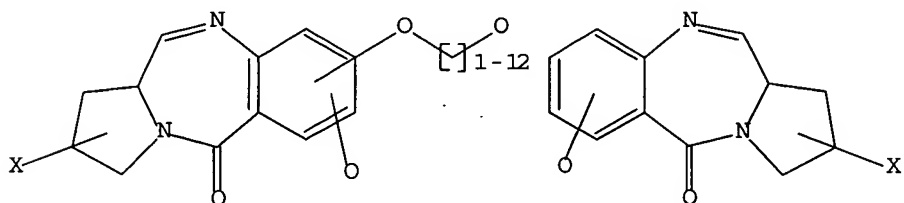
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L5 3 S L4

=> d l2; d his; log y

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.  
 L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 09:33:29 ON 27 JAN 2006)

FILE 'REGISTRY' ENTERED AT 09:34:02 ON 27 JAN 2006

L1 STRUCTURE UPLOADED  
 L2 QUE L1  
 L3 1 S L2  
 L4 8 S L2 FUL

FILE 'CAPLUS' ENTERED AT 09:34:28 ON 27 JAN 2006

L5

3 S L4

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	15.79	182.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

STN INTERNATIONAL LOGOFF AT 09:35:03 ON 27 JAN 2006